Claims

1. A hybrid learning system for searching an experimental space, comprising:

a data mart configured to acquire, store and manipulate at least, historical experimental data, descriptor data, and concurrent experimental data;

a search engine configured to use selection techniques to select a set of evaluation points representing a corresponding set of experiments to be run, based on the data from the data mart; and

a point evaluation mechanism configured with

(i) learning modules which perform predictive processing on the evaluation points selected by the search engine, and

(ii) a scoring module which performs a rating operation on outputs of the learning modules to rate the outputs of the learning modules,

wherein operation of the data mart, search engine and point evaluation mechanism are operated a plurality of times such that a repeating process is undertaken to obtain a finalized output.

2. The system according to claim 1 further including a physical experiment, wherein results of the physical experiment are supplied to the data mart.

3. The system according to claim 2 wherein the experimental space is a Combinatorial Chemistry experimental space.

4. The system according to claim 3 wherein an input to the system are experiments and the output of the system is a set of elements that yield a highest turnover number (TON) and selectivity.

5. A method for exploring an experimental space using a hybrid learning system, the method comprising:

(a) generating an experimental space including a plurality of experimental points, representing potential solutions to an experiment;

(b) collecting historical experimental data, descriptor data, and concurrent experimental data;

(c) storing the historical experimental data, descriptor data, and concurrent experimental data in a data mart, wherein the data mart includes the ability to be queried;

(d) performing a genetic algorithm processing loop on the experimental space to obtain a subset of experimental points from the plurality of experimental points;

(e) performing a clustering processing loop on the experimental space to obtain a subset of experimental points from the plurality of experimental points;

(f) selecting the subset of experimental points from at least one of the genetic algorithm processing step and the clustering processing step;

(g) supplying the selected experimental points and a subset of the data from the data mart to a point evaluation mechanism;

(h) performing a supervised learning process on the selected points; and

(i) obtaining an output.

6. The method of claim 5 further including performing a physical experiment using experimental points from the experimental space to obtain actual physical experimental results.

7. The method of claim 6 wherein the physical experimental results are supplied to the data mart.

8. The method according to claim 5 wherein steps (b) – (i) are repeated.

9. The method according to claim 5 wherein the experimental space is a Combinatorial Chemistry experimental space.

10. The method of claim 5 wherein the clustering loop includes:

(a) partitioning the experimental space into clusters of points having similarities;

(b) selecting a sample from each cluster, the sample being at least one evaluation point, wherein the selected samples are a first generation of evaluation points;

(c) performing at least one of actual physical experiments or synthetic models of experiments using the first generation of evaluation points;

(d) scoring each cluster based on an outcome of the at least actual experiment and synthetic models;

(e) selecting a cluster based on the scoring;

(f) repartitioning the experimental space into clusters on a reduced space; and

(g) repeating steps (b) – (f).

11. The method of claim 5 wherein genetic algorithm loop includes:

(a) partitioning the experimental space into uniform spaces of points;

(b) selecting a sample from each uniform space, the sample being at least one evaluation point, wherein the selected samples are a first generation of evaluation points;

(c) performing at least one of actual physical experiments or synthetic models of experiments using the first generation of evaluation points;

(d) scoring each uniform space based on an outcome of the at least actual experiment and synthetic models;

(e) selecting points to be parents based on the scoring;

(f) generating a next generation of points based on selected parents; and

(g) repeating steps (b) – (f).

12. The method according to claim 5 wherein each time a set of experiments is performed, additional data is added to the system and a further refined model is generated.

13. The method according to claim 5 wherein the selection processes are run against a new improved model.

14. A hybrid learning system for searching an experimental space comprising:

a data mart configured to receive, store and supply data;

a search engine including at least a genetic algorithm processor and a clustering processor configured to operate in parallel, both the genetic algorithm processor and the clustering processor configured to request data from the data mart, in order to select a set of points from the experimental space, the points representing a corresponding set of experiments to be undertaken; and

a point evaluation mechanism including at least one learning module and a scoring module, the at least one learning module receiving data from the data mart and the search engine and having a model experiment to which the selected points and data are applied.